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singular moment matrices**

**Part I: ML-Estimation of time series**

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# SEM modeling with singular moment matrices

## Part I: ML-Estimation of time series

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### Abstract

A structural equation model (SEM) with deterministic intercepts is introduced. The gaussian likelihood function does not contain determinants of sample moment matrices and is thus well defined for only one statistical unit. The SEM is applied to the dynamic state space model and compared with the Kalman filter (KF) approach. The likelihoods of both methods are shown to be equivalent, but for long time series numerical problems occur in the SEM approach, which are traced to the inversion of the latent state covariance matrix. Both approaches are compared on several aspects. The SEM approach is now open for idiographic analysis and estimation of panel data with correlated units.

**Key Words:** Structural Equation Models (SEM); Time series; Kalman Filtering (KF); State Space Models; Maximum Likelihood (ML) Estimation.

## 1 Introduction

Structural equation models (SEM) are well known and widely applied tools of specifying multivariate relations between latent states and their measured indicators. Usually one considers cross sectional data and analyzes the relations of a latent  $p$ -vector  $\eta_n$ , measured with independent replications of the indicators  $y_n$ ,  $n = 1, \dots, N$ . In the case of panel data  $y_{nt}$ ,  $t = 0, \dots, T$  one can fill the time series for each panel unit into the components of the indicators and analyze

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the time dependence as a multivariate vector (cf., e.g. Möbus and Nagl; 1983; Oud et al.; 1993; Arminger and Müller; 1990).

However, in the time series case ( $N = 1$ ) an apparent problem occurs: The sample moment matrix is singular, since only one observation vector  $y = \{y_{10}, \dots, y_{1T}\}$  is present. Nevertheless, the theory of time series analysis and Kalman filtering shows (cf., e.g. Schweppe; 1965; Jazwinski; 1970; Caines; 1988), that the likelihood function is well defined and ML estimates can be computed. There were attempts to create artificial samples with  $N > 1$  by layering pieces of the time series in the data matrix, but then the statistical units  $n$  are dependent. In this paper it is shown that such procedures are not necessary at all, since the likelihood function of a SEM is well defined even for  $N = 1$  (cf. also Singer; 2007). In some well known programs ML fit functions are used which depend on the log determinant of the singular moment matrix, but these terms do not occur in the exact likelihood.

The likelihood computed by the SEM is compared with the likelihood obtained recursively by the Kalman filter (KF) and both procedures yield identical results. For long time series and panels, there are numerical differences, since the SEM involves matrices of order  $(T+1)p \times (T+1)p$ , whereas the KF only uses matrices of order  $p \times p$ , where  $p$  is the dimension of the latent state component  $\eta_{nt}$ .

This will be detailed in the further sections. Section 2 gives the definition of a SEM model including deterministic intercept terms and states the Gaussian likelihood function. In section 3 the case of time series data with measurement error is treated. The likelihood function of the SEM representation is explicitly transformed to the prediction error decomposition and numerical differences are detected. In an appendix, computational aspects are shortly discussed.

## 2 SEM modeling

In the following the SEM model

$$\eta_n = B\eta_n + \Gamma x_n + \zeta_n \quad (1)$$

$$y_n = \Lambda\eta_n + \tau x_n + \epsilon_n \quad (2)$$

$n = 1, \dots, N$ , will be considered. The structural matrices have dimensions  $B : P \times P$ ,  $\Gamma : P \times Q$ ,  $\Lambda : K \times P$ ,  $\tau : K \times Q$  and  $\zeta_n \sim N(0, \Sigma_\zeta)$ ,  $\epsilon_n \sim N(0, \Sigma_\epsilon)$  are independent normally distributed error terms ( $\Sigma_\zeta : P \times P$ ,  $\Sigma_\epsilon : K \times K$ ).

In the structural and the measurement model, the variables  $x_n$  are *deterministic* control variables. They can be used to model intercepts and for dummy coding. Stochastic exogenous variables  $\xi_n$  are included by extending the latent variables

$\eta_n$ . For example, the LISREL model with intercepts is obtained as

$$\begin{aligned} \begin{bmatrix} \eta_n \\ \xi_n \end{bmatrix} &= \begin{bmatrix} B & \Gamma \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \eta_n \\ \xi_n \end{bmatrix} + \begin{bmatrix} \alpha \\ \kappa \end{bmatrix} \mathbf{1} + \begin{bmatrix} \zeta_n \\ \tilde{\zeta}_n \end{bmatrix} \\ \begin{bmatrix} y_n \\ x_n \end{bmatrix} &= \begin{bmatrix} \Lambda_y & 0 \\ 0 & \Lambda_x \end{bmatrix} \begin{bmatrix} \eta_n \\ \xi_n \end{bmatrix} + \begin{bmatrix} \tau_y \\ \tau_x \end{bmatrix} \mathbf{1} + \begin{bmatrix} \epsilon_n \\ \delta_n \end{bmatrix} \\ \text{Var} \begin{pmatrix} \zeta_n \\ \tilde{\zeta}_n \end{pmatrix} &= \begin{bmatrix} \Psi & 0 \\ 0 & \Phi \end{bmatrix} \\ \text{Var} \begin{pmatrix} \epsilon_n \\ \delta_n \end{pmatrix} &= \begin{bmatrix} \Sigma_\epsilon & 0 \\ 0 & \Sigma_\delta \end{bmatrix}. \end{aligned}$$

Since the error vectors are normally distributed, the indicators (2) are distributed as  $N(\mu_{y_n}, \Sigma_y)$ , where

$$\eta_n = B_1(\Gamma x_n + \zeta_n) \quad (3)$$

$$E[\eta_n] = B_1 \Gamma x_n \quad (4)$$

$$\text{Var}(\eta_n) = B_1 \Sigma_\zeta B_1' \quad (5)$$

$$E[y_n] = \mu_{y_n} = \Lambda E[\eta_n] + \tau x_n = [\Lambda B_1 \Gamma + \tau] x_n := C x_n \quad (6)$$

$$\text{Var}[y_n] = \Sigma_y = \Lambda \text{Var}(\eta_n) \Lambda' + \Sigma_\epsilon = \Lambda B_1 \Sigma_\zeta B_1' \Lambda' + \Sigma_\epsilon. \quad (7)$$

In the equations above, it is assumed that  $B_1 := (I - B)^{-1}$  exists. Thus, the log likelihood function for the  $N$  observations  $\{y_n, x_n\}$  is

$$l = -\frac{N}{2} \left( \log |\Sigma_y| + \text{tr} \left[ \Sigma_y^{-1} \frac{1}{N} \sum_n (y_n - \mu_{y_n})(y_n - \mu_{y_n})' \right] \right).$$

Inserting  $\mu_{y_n}$  (eqn. 6) and using the data matrices  $Y' = [y_1, \dots, y_N] : K \times N$ ,  $X' = [x_1, \dots, x_N] : Q \times N$ , the log likelihood is

$$l = -\frac{N}{2} (\log |\Sigma_y| + \text{tr} [\Sigma_y^{-1} (M_y + C M_x C' - M_{yx} C' - C M_{xy})]), \quad (8)$$

with the moment matrices  $M_y = Y'Y : K \times K$ ,  $M_x = X'X : Q \times Q$ ,  $M_{yx} = Y'X : K \times Q$ .

In order to implement arbitrary restrictions on the structural matrices, it is assumed that they depend on an  $u$ -dimensional parameter vector  $\psi$ , e.g.  $\Sigma_\zeta = \Sigma_\zeta(\psi)$  etc. For example, setting  $\Sigma_\zeta = G(\psi)G(\psi)'$  with  $G =$  lower triangular matrix, the structural error covariance is positive semidefinite. Another example is the use of the matrix exponential function in the definition of the exact discrete model (Singer; 2009).

The likelihood function (8) is well defined for  $N = 1$ , since no log determinants of the sample moment matrices are involved, as is suggested by the ML fitting function of LISREL (cf. LISREL 8 reference guide, p. 21, eqns. 1.14, 1.15, p.

298, eqn. 10.8). The covariance matrix of the indicators,  $\Sigma_y$  (eqn. 7), must be nonsingular, however.<sup>1</sup>

In order to make the discussion more transparent and explicit, the representation of time series as SEM will be considered.

### 3 Time series and SEM modeling

#### 3.1 SEM representation of a dynamical state space model

The discrete time dynamical state space model (vector autoregression VAR(1) with measurement model) is defined by

$$y_{i+1} = \alpha_i y_i + \beta_i x_i + u_i; \quad i = 0, \dots, T-1 \quad (9)$$

$$z_i = H_i y_i + D_i x_i + \epsilon_i; \quad i = 0, \dots, T \quad (10)$$

with independent Gaussian errors  $E[u_i] = 0, \text{Var}(u_i) = \Omega, E[\epsilon_i] = 0, \text{Var}(\epsilon_i) = R_i$ . The dimensions of the dynamic structural matrices are  $\alpha_i : p \times p, \beta_i : p \times q, \Omega_i : p \times p, H_i : k \times p, D_i : k \times q, R_i : k \times k$ . The initial distribution is assumed to be  $y_0 \sim N(\mu, \Sigma)$  independent of  $u_0$  and  $x_i$  are deterministic control variables.

This model is very general and permits the treatment of ARIMAX models, dynamic factor analysis, colored noise models etc. (Akaike; 1974; Watson and Engle; 1983; Caines; 1988). All structural matrices depend on a parameter vector  $\psi$ .<sup>2</sup>

It can be treated recursively by the Kalman filter or simultaneously by the matrix equation ( $N = 1$ )

$$\eta = B\eta + \Gamma x + \zeta \quad (11)$$

$$y = \Lambda\eta + \tau x + \epsilon, \quad (12)$$

where  $\eta' = [y'_0, \dots, y'_T] : 1 \times (T+1)p$  is the latent state,  $\zeta' = [\zeta'_0, u'_0, \dots, u'_{T-1}] : 1 \times (T+1)p$  is a vector of process errors,  $y' = [z'_0, \dots, z'_T] : 1 \times (T+1)k$  are the measurements and  $x' = [1, x'_0, \dots, x'_T] : 1 \times (1 + (T+1)q)$  are (deterministic) exogenous variables.

<sup>1</sup>Otherwise the singular normal distribution can be used (Mardia et al.; 1979, p. 41).

<sup>2</sup> Moreover, the system matrices may depend on lagged measurements  $Z^i = \{z_i, \dots, z_0\}$ , and the measurement matrices  $H_i, d_i, R_i$  on  $Z^{i-1}$  in order to specify ARCH effects. This so called *conditional Gaussian model* can be treated by the Kalman filter (Liptser and Shirayev; 2001, vol. II), but not by SEM.

The structural matrices are (system model)

$$B = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ \alpha_0 & 0 & 0 & \dots & 0 \\ 0 & \alpha_1 & 0 & \dots & 0 \\ \vdots & 0 & \ddots & 0 & 0 \\ 0 & 0 & \dots & \alpha_{T-1} & 0 \end{bmatrix}$$

$$\Gamma = \begin{bmatrix} \mu & 0 & 0 & 0 & \dots & 0 \\ 0 & \beta_0 & 0 & 0 & \dots & 0 \\ 0 & 0 & \beta_1 & 0 & \dots & 0 \\ \vdots & 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & \beta_{T-1} & 0 \end{bmatrix}$$

$$\text{Var}(\zeta) = \Sigma_\zeta = \begin{bmatrix} \Sigma & 0 & 0 & \dots & 0 \\ 0 & \Omega_0 & 0 & \dots & 0 \\ 0 & 0 & \Omega_1 & \dots & 0 \\ \vdots & 0 & 0 & \ddots & 0 \\ 0 & 0 & \dots & 0 & \Omega_{T-1} \end{bmatrix}.$$

Furthermore

$$\Lambda = \begin{bmatrix} H_0 & 0 & 0 & \dots & 0 \\ 0 & H_1 & 0 & \dots & 0 \\ 0 & 0 & H_2 & \dots & 0 \\ \vdots & 0 & 0 & \ddots & 0 \\ 0 & 0 & \dots & 0 & H_T \end{bmatrix}$$

$$\tau = \begin{bmatrix} 0 & D_0 & 0 & 0 & \dots & 0 \\ 0 & 0 & D_1 & 0 & \dots & 0 \\ 0 & 0 & 0 & D_2 & 0 & 0 \\ \vdots & \dots & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & D_T \end{bmatrix}$$

$$\text{Var}(\epsilon) = \Sigma_\epsilon = \begin{bmatrix} R_0 & 0 & 0 & \dots & 0 \\ 0 & R_1 & 0 & \dots & 0 \\ 0 & 0 & R_2 & \dots & 0 \\ \vdots & \vdots & 0 & \ddots & 0 \\ 0 & 0 & \dots & 0 & R_T \end{bmatrix}$$

are the factor loading, *deterministic* intercept and error parameter matrices of the measurement model. If there are missing data present in  $z_i$ , the respective rows in  $\Lambda$  are dropped (cf. example sect. 3.4).

Solving for  $\eta$  one obtains the solution of the VAR(1) (eqn. 9) for the time points  $t_i$

$$\eta = (I - B)^{-1}(\Gamma x + \zeta). \quad (13)$$

In this equation, the initial condition is represented by  $\eta_0 = y(t_0) = \mu + \zeta_0 \sim N(\mu, \Sigma)$ . This may be seen more explicitly by noting that

$$(I - B)^{-1} = \sum_{l=0}^T B^l = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ \alpha_0 & 1 & 0 & \dots & 0 & 0 \\ \alpha_1 \alpha_0 & \alpha_1 & 1 & 0 & \dots & 0 \\ \dots & \dots & \dots & \ddots & \dots & \dots \\ \alpha_{T-2} \alpha_{T-3} \dots \alpha_0 & \alpha_{T-2} \alpha_{T-3} \dots \alpha_1 & \dots & \alpha_{T-2} & 1 & 0 \\ \alpha_{T-1} \alpha_{T-2} \dots \alpha_0 & \alpha_{T-1} \alpha_{T-2} \dots \alpha_1 & \dots & \dots & \alpha_{T-1} & 1 \end{bmatrix}$$

since  $B$  is nilpotent ( $B^l = 0; l > T$ ). For example, setting  $T = 4$  one obtains

$$(I - B)^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \alpha_0 & 1 & 0 & 0 & 0 \\ \alpha_1 \alpha_0 & \alpha_1 & 1 & 0 & 0 \\ \alpha_2 \alpha_1 \alpha_0 & \alpha_2 \alpha_1 & \alpha_2 & 1 & 0 \\ \alpha_3 \alpha_2 \alpha_1 \alpha_0 & \alpha_3 \alpha_2 \alpha_1 & \alpha_3 \alpha_2 & \alpha_3 & 1 \end{bmatrix}.$$

Inserting in eqn. (13) one can compute the explicit solution of (9), in components

$$\begin{aligned} y_0 &= \mu + \zeta_0 \sim N(\mu, \Sigma) \\ y_i &= \left( \prod_{l=i-1}^0 \alpha_l \right) y_0 + \sum_{j=0}^{i-1} \left( \prod_{l=0, l \geq 0}^{i-j-2} \alpha_{i-1-l} \right) (\beta_j x_j + u_j), \\ i &= 1, \dots, T, \end{aligned} \quad (14)$$

where the time ordering must be respected ( $\alpha_i$  left of  $\alpha_j$  for times  $i > j$ ). In the special case of constant  $\alpha$  one gets the familiar form

$$y_i = \alpha^i y_0 + \sum_{j=0}^{i-1} \alpha^{i-j-1} (\beta_j x_j + u_j).$$

## 3.2 Likelihood function with singular moment matrices

If the structural matrices do not depend on measurements  $z_i$  (see footnote 2), the system is multivariate Gaussian and the log likelihood function reads

$$l = -\frac{1}{2} (\log |\Sigma_y| + \text{tr} [\Sigma_y^{-1} (M_y + C M_x C' - M_{yx} C' - C M_{xy})]), \quad (15)$$

with the singular moment matrices  $M_y = yy' : K \times K$ ,  $M_x = xx' : Q \times Q$ ,  $M_{yx} = yx' : K \times Q$  and  $K = (T + 1)k$ ,  $Q = (T + 1)q + 1$  and  $C = \Lambda B_1 \Gamma + \tau$ .

### 3.2.1 Likelihood function without measurement model

In the special case without measurement model ( $y = \eta$ ), the likelihood may be simplified using

$$\Sigma_y = B_1 \Sigma_\zeta B_1'$$

and thus

$$l = -\frac{1}{2}(\log |\Sigma_\zeta| + \text{tr} [\Sigma_\zeta^{-1}(I - B)(y - \mu_y)(y - \mu_y)'(I - B)']),$$

where it has been used that  $|I - B| = 1$  and  $\text{tr}[AB] = \text{tr}[BA]$ . Noting that  $\mu_y = B_1 \Gamma x$ , we find

$$\begin{aligned} l &= -\frac{1}{2}(\log |\Sigma_\zeta| + \text{tr} [\Sigma_\zeta^{-1}[(I - B)y - \Gamma x][(I - B)y - \Gamma x]']) \\ &= -\frac{1}{2}(\log |\Sigma_\zeta| + \text{tr} [\Sigma_\zeta^{-1} \zeta \zeta']). \end{aligned}$$

Using the special structure of  $B$  we obtain  $\zeta_0 = y_0 - \mu$ ,  $\zeta_{i+1} = y_{i+1} - \alpha_i y_i - \beta_i x_i$ ,  $i = 0, \dots, T - 1$ . Inserting the blockdiagonal form of  $\Sigma_\zeta$  one gets the explicit result

$$\begin{aligned} l &= -\frac{1}{2}(\log |\Sigma| + \text{tr}[\Sigma^{-1}(y_0 - \mu)(y_0 - \mu)']) \\ &\quad + \sum_{i=0}^{T-1} \log |\Omega_i| + \text{tr} [\Omega_i^{-1}(y_{i+1} - \alpha_i y_i - \beta_i x_i)(y_{i+1} - \alpha_i y_i - \beta_i x_i)']. \end{aligned} \quad (16)$$

But this is the prediction error decomposition of the likelihood which is directly obtained from the dynamical model (9). One can write

$$\begin{aligned} E[y_{i+1}|y_i] &= \alpha_i y_i + \beta_i x_i \\ \text{Var}(y_{i+1}|y_i) &= \Omega_i \end{aligned}$$

and thus, using the Markov property of  $y_i$ ,

$$l = \log p(y_T, \dots, y_0) = \log[p(y_T|y_{T-1}) \dots p(y_1|y_0)p(y_0)] \quad (17)$$

$$= \log p(y_0) + \sum_{i=0}^{T-1} \log p(y_{i+1}|y_i), \quad (18)$$

where  $p(y_{i+1}|y_i) = \phi(y_{i+1}; \alpha_i y_i + \beta_i x_i, \Omega_i)$  (conditional normal distribution) and  $p(y_0) = \phi(y_0; \mu, \Sigma)$ . Up to constants ( $\propto \log 2\pi$ ) the expressions (16) and (18) coincide.



### 3.2.2 Likelihood function with measurement model

In this case the likelihood

$$\begin{aligned} p(y) &= p(z_T, \dots, z_0) \\ &= |2\pi\Sigma_y|^{-1/2} \exp(-\frac{1}{2}\text{tr}[\Sigma_y^{-1}(y - \mu_y)(y - \mu_y)']) \\ \mu_y &= (\Lambda B_1 \Gamma + \tau)x \\ \Sigma_y &= \Lambda B_1 \Sigma_\zeta B_1' \Lambda' + \Sigma_\epsilon \end{aligned}$$

cannot be decomposed into  $p(z_T|z_{T-1}) \dots p(z_1|z_0)$ , since  $z_i$  is not Markovian due to the measurement model [i.e.  $p(z_i|z_{i-1}, \dots, z_0) \neq p(z_i|z_{i-1})$ ]. This may be seen as follows:

Using the Bayes formula one can condition on earlier measurements  $Z^i = \{z_i, \dots, z_0\}$  and write

$$\begin{aligned} p(y) &= p(z_T, \dots, z_0) \\ &= p(z_T|z_{T-1}, \dots, z_0) p(z_{T-1}, \dots, z_0) \\ &= \prod_{i=0}^{T-1} p(z_{i+1}|Z^i) p(z_0). \end{aligned}$$

Since  $y = \{z_0, \dots, z_T\}$  is a Gaussian system, the conditional distributions are Gaussian as well with parameters (see eqn. 10)

$$\begin{aligned} E[z_{i+1}|Z^i] &= H_{i+1}E[y_{i+1}|Z^i] + D_{i+1}x_{i+1} \\ \text{Var}(z_{i+1}|Z^i) &= H_{i+1}\text{Var}(y_{i+1}|Z^i)H_{i+1}' + R_{i+1}. \end{aligned}$$

This is the optimal prediction of  $z_{i+1}$  in the mean square sense using the information set  $Z^i$ , with error covariance  $\text{Var}(z_{i+1}|Z^i)$ .

The conditional expectations of the latent variables  $y_i$  can be computed recursively using the dynamical model (9)

$$\begin{aligned} E[y_{i+1}|Z^i] &= \alpha_i E[y_i|Z^i] + \beta_i x_i \\ \text{Var}(y_{i+1}|Z^i) &= \alpha_i \text{Var}[y_i|Z^i] \alpha_i' + \Omega_i \\ i &= 0, \dots, T-1 \end{aligned}$$

since  $\text{Var}(u_i|Z^i) = \Omega_i$  (this may depend on  $Z^i$ ). The recursion is usually abbreviated as:

*time update, a priori moments:*

$$\mu_{i+1|i} = \alpha_i \mu_{i|i} + \beta_i x_i \quad (19)$$

$$\Sigma_{i+1|i} = \alpha_i \Sigma_{i|i} \alpha_i' + \Omega_i \quad (20)$$

$$i = 0, \dots, T-1.$$

The equal time (a posteriori) expectations are given in terms of earlier a priori moments (theorem on normal correlation, Liptser and Shirayev (2001, vol. II); see eqn. 30):

*measurement update, a posteriori moments:*

$$\mu_{i|i} = \mu_{i|i-1} + \Sigma_{i|i-1} H_i' \Gamma_i^- \nu_i \quad (21)$$

$$\Sigma_{i|i} = \Sigma_{i|i-1} - \Sigma_{i|i-1} H_i' \Gamma_i^- H_i \Sigma_{i|i-1} \quad (22)$$

$$\nu_i := z_i - (H_i \mu_{i|i-1} + D_i x_i) \quad (23)$$

$$\Gamma_i := H_i \Sigma_{i|i-1} H_i' + R_i \quad (24)$$

$$i = 0, \dots, T - 1.$$

( $\Gamma_i^-$  = pseudo(g)-inverse if singular). The prediction error and its conditional covariance matrix (filter error covariance)

$$\nu_i = z_i - E[z_i | Z^{i-1}]$$

$$\Gamma_i := \text{Var}(z_i | Z^{i-1})$$

are obtained by the time update formulas (19–20).

The iteration is started with the

*initial condition:*

$$\mu_{0|0} = \mu_{0|-1} + \Sigma_{0|-1} H_0' \Gamma_0^- \nu_0$$

$$\Sigma_{0|0} = \Sigma_{0|-1} - \Sigma_{0|-1} H_0' \Gamma_0^- H_0 \Sigma_{0|-1}$$

$$\nu_0 := z_0 - (H_0 \mu_{0|-1} + D_0 x_0)$$

$$\Gamma_0 := H_0 \Sigma_{0|-1} H_0' + R_0$$

and setting the expectations  $\mu_{0|-1} = E[y_0] = \mu$ ,  $\Sigma_{0|-1} = \text{Var}[y_0] = \Sigma$  equal to the initial conditions of the latent state  $y_0$ . This is because at time  $i = 0$  we just have the information in  $z_0$ , but no presample information  $z_{-1}, \dots$ . Thus we have derived the

*Kalman filter algorithm:*

initial condition	$\mu_{0 0}, \Sigma_{0 0}$
likelihood	$p(z_0) = \phi(z_0; E[z_0], \text{Var}(z_0))$
recursion	$i = 0, \dots, T - 1$
time update	$\mu_{i+1 i}, \Sigma_{i+1 i}$
measurement update	$\mu_{i+1 i+1}, \Sigma_{i+1 i+1}$
likelihood	$p(z_{i+1}   Z^i) = \phi(z_{i+1}; E[z_{i+1}   Z^i], \text{Var}(z_{i+1}   Z^i))$

It is a sequence of extrapolation steps (time update) and measurement updates (normal correlation) in order to compute the conditional moments

$$\begin{aligned} E[z_{i+1}|Z^i] &= H_{i+1}\mu_{i+1|i} + D_{i+1}x_{i+1} \\ \text{Var}(z_{i+1}|Z^i) &= H_{i+1}\Sigma_{i+1|i}H'_{i+1} + R_{i+1}. \end{aligned}$$

for the likelihood function  $\phi(z_{i+1}; E[z_{i+1}|Z^i], \text{Var}(z_{i+1}|Z^i))$  of measurement  $z_{i+1}$ . From the recursions it is seen that all earlier measurements are contained in the conditional moments, thus  $z_i$  is not Markovian. Nevertheless, the likelihood in the prediction error decomposition has a simple structure, since the prediction errors are uncorrelated<sup>3</sup>, i.e.

$$p(z_T, \dots, z_0) = \prod_{i=0}^{T-1} p(z_{i+1}|Z^i)p(z_0) \quad (25)$$

$$= \prod_{i=0}^{T-1} \phi(z_{i+1}; E[z_{i+1}|Z^i], \text{Var}(z_{i+1}|Z^i))p(z_0) \quad (26)$$

$$= \prod_{i=0}^{T-1} \phi(\nu_{i+1}; 0, \Gamma_{i+1})p(z_0). \quad (27)$$

with initial distribution  $p(z_0) = \phi(z_0; E[z_0], \text{Var}(z_0)) = \phi(z_0; H_0\mu + D_0x_0, H_0\Sigma H'_0 + R_0)$ .

In the case without measurement model ( $z_i = y_i$ ), one recovers the Markovian structure  $\nu_{i+1} = y_{i+1} - E[y_{i+1}|Y^i] = y_{i+1} - E[y_{i+1}|y_i]; \Gamma_{i+1} = \Omega_{i+1}$  (cf. eqn. 17).

### 3.3 Numerical example: AR(2) time series with measurement error

In order to facilitate the theoretical discussion with a practical example, an autoregressive time series of the form

$$\begin{aligned} y_{i+2} &= \phi_1 y_{i+1} + \phi_2 y_i + \beta + u_i; \quad i = 0, \dots, T-1 \\ z_i &= y_i + \epsilon_i; \quad i = 0, \dots, T \end{aligned}$$

is considered. In state space form this reads

$$\begin{bmatrix} y_{i+1} \\ y_{i+2} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \phi_2 & \phi_1 \end{bmatrix} \begin{bmatrix} y_i \\ y_{i+1} \end{bmatrix} + \begin{bmatrix} 0 \\ \beta \end{bmatrix} 1 + \begin{bmatrix} 0 \\ u_i \end{bmatrix}; \quad i = 0, \dots, T-1 \quad (28)$$

$$z_i = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} y_i \\ y_{i+1} \end{bmatrix} + \epsilon_i; \quad i = 0, \dots, T \quad (29)$$

<sup>3</sup>The prediction errors  $\nu_{i+1} = z_{i+1} - E[z_{i+1}|Z^i]$  are martingale differences, i.e.  $E[\nu_{i+1}|Z^i] = 0$  and thus uncorrelated, since for  $i > j$  we have  $E[\nu_i \nu'_j] = E[E[\nu_i \nu'_j | Z^{i-1}]] = E[E[\nu_i | Z^{i-1}] \nu'_j] = 0$ .

For system matrices independent of the measurements they are Gaussian and thus even independent (cf. Liptser and Shirayev, loc. cit., ch. 13)

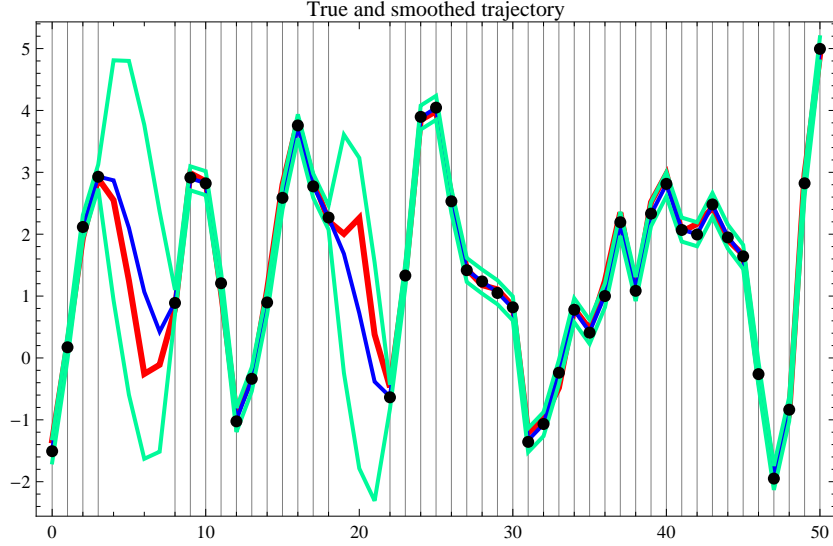


Figure 1: AR(2) time series with missing data ( $T = 50$ ): Measurements  $z_i$  (dots), true trajectory  $y_i$  (red) and smoothed states  $E[y_i|Z^T]$  (blue). Also displayed are 95% HPD confidence bands  $E[y_i|Z^T] \pm 1.96 \cdot \text{Std}[y_i|Z^T]$ (green).

The parameter values were chosen as  $\phi_1 = 1, \phi_2 = -.5, \beta = 1, \Omega = \text{Var}(u_i) = 1 = g^2, R = \text{Var}(\epsilon_i) = 10^{-2}$ . The initial condition is distributed as  $[y_0, y_1] \sim N([0, 0], \text{diag}(1, 1))$ . The eigenvalues of the structural matrix  $\alpha$  are the solutions of

$$|\alpha - \lambda I| = 0 = -\lambda(\phi_1 - \lambda) - \phi_2,$$

$$\lambda_{1,2} = \phi_1/2 \pm \sqrt{\phi_1^2/4 + \phi_2} = 1/2 \pm i/2 = r(\cos \omega + i \sin \omega).$$

Thus one obtains a stationary process with damped oscillations of angular frequency  $\omega_{1,2} = \pm\pi/4$  and period  $T_o = 2\pi|\omega_{1,2}| = 8$ .

The dynamic state space model (28) was represented as a SEM model and the measured and latent data  $(y, \eta)$  were simulated from this system. Fig. 1 shows the data  $z_i$  (dots), the true trajectory  $y_i$  (red) and smoothed states  $E[y_i|Z^T]$  (blue), together with 95% HPD<sup>4</sup> confidence bands  $E[y_i|Z^T] \pm 1.96 \cdot \text{Std}[y_i|Z^T]$ (green). It was assumed that at times  $i = \{4, 5, 6, 7, 19, 20, 21\}$  the data are missing. This is reflected in the figure by larger confidence bands. The smoothed trajectory was computed from the SEM by using the *theorem on normal correlation*

$$E[\eta|y] = E[\eta] + \text{Cov}(\eta, y)\text{Var}(y)^-(y - E[y]) \quad (30)$$

$$\text{Var}[\eta|y] = \text{Var}[\eta] - \text{Cov}(\eta, y)\text{Var}(y)^-\text{Cov}(y, \eta). \quad (31)$$

( $\text{Var}(y)^- = \text{pseudo}(g)\text{-inverse}$ ).

<sup>4</sup>highest posterior probability

parameters	SEM			SEM (g-inverse)		KF	
	<i>true</i>	$\hat{\psi}$	std	$\hat{\psi}$	std	$\hat{\psi}$	std
$\phi_2$	-0.5	-0.411829	0.203714	-0.411829	0.203711	-0.411776	0.203713
$\phi_1$	1	0.904962	0.206195	0.904962	0.206194	0.904894	0.206186
$b$	1	1.2662	0.451959	1.2662	0.451951	1.26624	0.451983
$g$	1	1.1797	0.194988	1.1797	0.194988	1.17979	0.194974
<i>lik</i>		-13.232880492509315		-13.232880492509263		-13.232982394747465	

Table 1: AR(2) model,  $T = 20$ . Comparison of SEM and KF ML-estimates and likelihood. The results for  $T = 50, T = 100$  are similar.

This corresponds to the regression estimator of Thompson in factor analysis. In figure 1, the true parameter values were used.

They can be estimated by maximum likelihood using the SEM likelihood (15) or by the prediction error decomposition (25) using the Kalman filter. The results for  $T = 20, T = 50$  and  $T = 100$  are very similar (cf. table 1 for  $T = 20$ ). There are small numerical differences, especially in the standard errors computed from the Hessian  $H = l_{\psi\psi}$  at the ML estimate  $\hat{\psi}$ , i.e.  $\widehat{\text{Var}}(\hat{\psi}) \approx (-H)^{-1}$ .

It is interesting to investigate the likelihood surface  $l(\psi)$  for several sample sizes  $T$ , since the dimensions of the SEM matrices are proportional to  $(T + 1)p$  and  $(T + 1)k$  ( $p = 2, k = 1$ ). Indeed, as fig. 2 shows for parameter  $\phi_2$ , there are numerical problems for parameter values far from the true ones, which are stronger for larger sample size. In contrast, the Kalman filter likelihood is always well behaved since only  $k \times k$  matrices must be inverted. The use of the g-inverse  $\Sigma_y^-$  does not improve the results, in fig. 2,  $T = 50$  (middle), they are even worse. Nevertheless, near the true values, the likelihoods are very similar and almost the same estimates are obtained.

The numerical problems can be traced to very large as well as negative and complex eigenvalues for the covariance matrix  $\Sigma_y$  of the observations (starting with  $\phi_2 > \approx .5, < \approx -1.5, T = 50$ ), which is positive semidefinite theoretically (figure 3). In the likelihood function, the determinant and the inverse is computed. A variant uses the singular normal distribution, where the product of positive eigenvalues and the g-inverse is used for the Gaussian density (Mardia et al.; 1979, p. 41).

### 3.4 Discussion

In this section the results of SEM vs. KF in time series analysis ( $N = 1$ ) will be summarized.

- Kalman Filter:
  - + The use of the recursive structure of the dynamical model leads to a decoupled 'white noise form' of the likelihood, where only matrices of

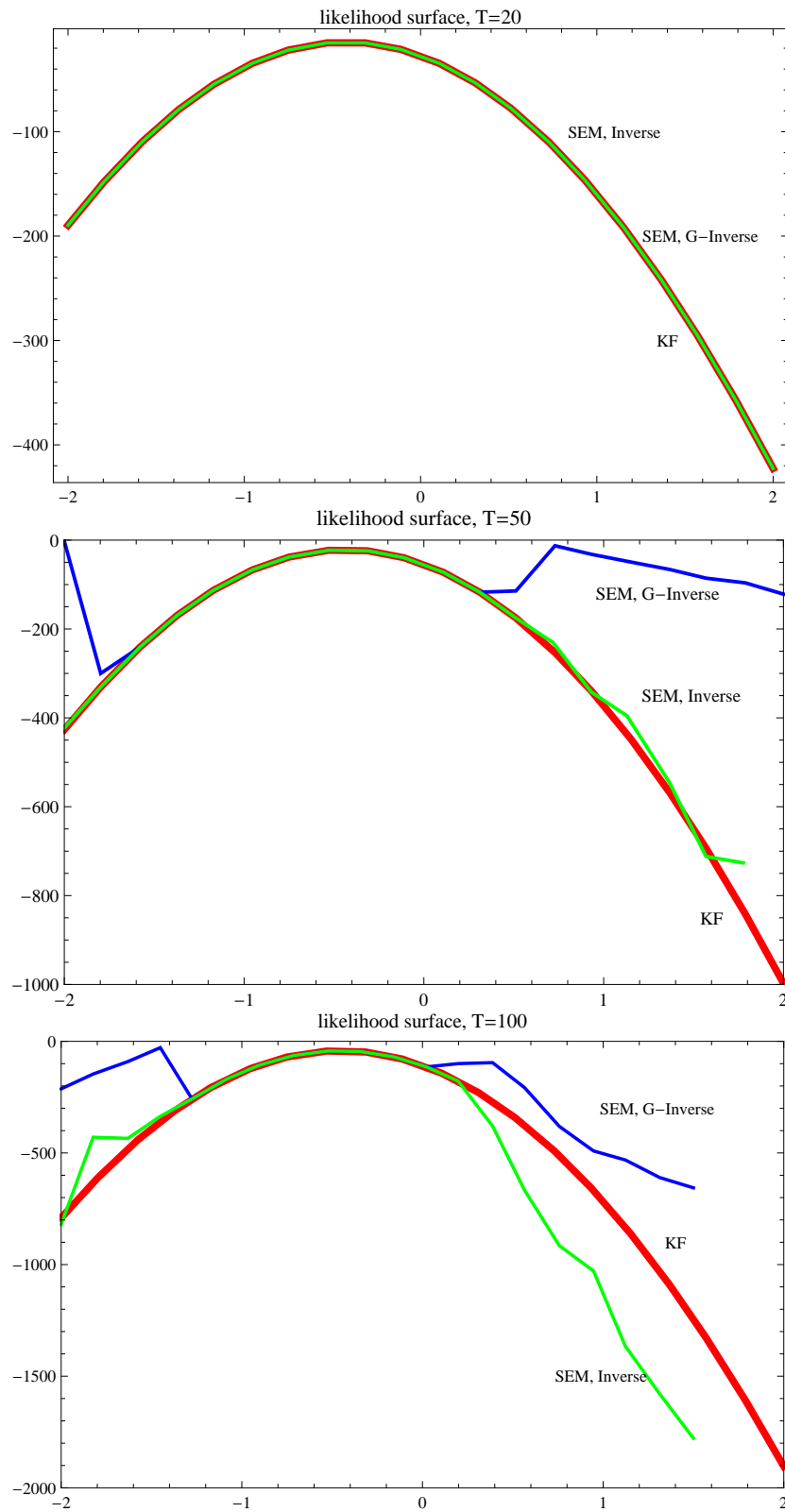


Figure 2: AR(2) time series: comparison of likelihood surface  $l(\phi_2)$  for sample sizes  $T = 20, 50, 100$ . SEM (inverse /g-inverse) vs. KF. The true value is  $\phi_2 = -0.5$ .

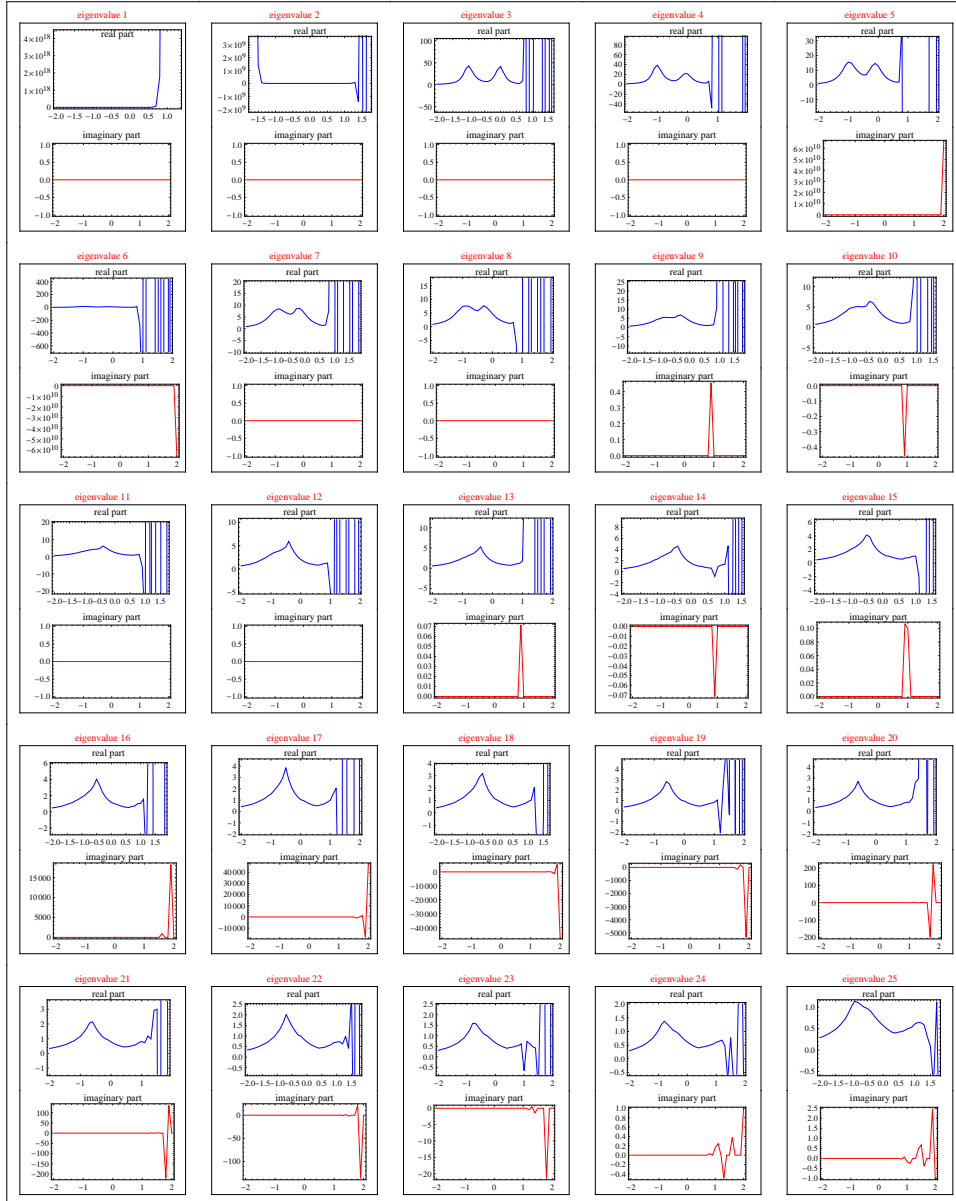
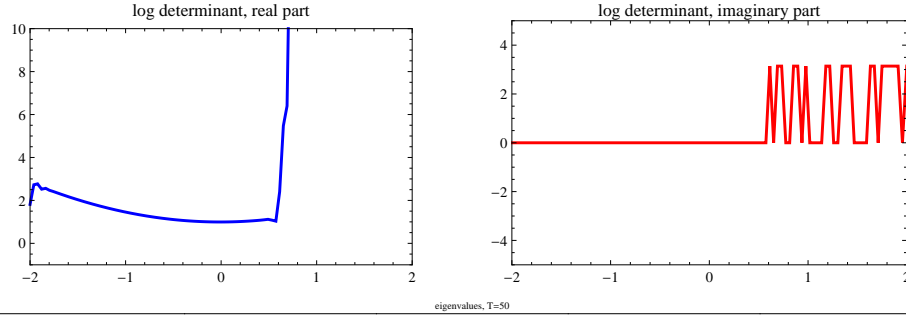


Figure 3: AR(2) time series,  $T = 50$ : log determinant  $\log(\det(\Sigma_y(\phi_2)))$  (top) and the first 25 eigenvalues of  $\Sigma_y(\phi_2)$ . One detects very large as well as complex and negative values, although the matrix is positive semidefinite theoretically.

order  $k \times k$  and  $p \times p$  are involved. Thus numerical problems are of smaller size.

- + One can compute the outer product of gradients (OPG) form of the Fisher information matrix,  $F = \sum_{i=0}^T E[s_i s_i']$ ;  $s_i = \partial l(z_i | Z^{i-1}) / \partial \psi$ , which may be used for the asymptotic standard errors, including the sandwich form  $J^{-1} F J^{-1}$  ( $J = -\partial^2 l / \partial \psi \psi' =$  observed information matrix) when misspecification is present; e.g. nongaussian data, but using likelihood (25).
- + The recursive form allows the treatment of conditionally Gaussian models, where the parameter matrices depend on lagged measurements. Thus a state space treatment of ARCH models is possible.
  - Recursive implementation can lead to performance loss in interpreter languages.
  - In the panel case  $N > 1$  the Kalman recursions must be computed for all units  $n = 1, \dots, N$ , although there are simplifications possible (matrix recursions for all filter states; the variances are independent of the data, etc; cf. Singer (1991, 1993)).

- SEM:

- + One can use matrix expressions, which is an advantage in interpreter languages (loops are slow). Moreover, the usage of several processor kernels is sometimes supported in the linear algebra routines (e.g. Mathematica).
- + In the panel case the likelihood depends on moment matrices, which are computed only once.
- + Time series models not fitting to the VAR scheme are easily specified. Moreover, multivariate models can be estimated for  $N = 1$ , if enough restrictions are present (idiographic analysis).
  - Large matrices of order  $k(T + 1) \times k(T + 1)$  must be inverted which can be problematic.
  - If the missing data structure is dependent on the panel unit, moment matrices cannot be used any more. Instead, in the individual likelihood approach, each panel unit must be treated separately leading to degraded performance.
  - Conditionally Gaussian models cannot be treated, since the joint distribution of all observations is not Gaussian anymore.



## 4 Conclusion

It has been shown that the representation of a dynamic state space model in terms of SEM leads to a well defined likelihood function, even for only one panel unit (time series case). More generally, multivariate models not fitting to the VAR(1) scheme can be estimated on  $N = 1$  (idiographic analysis), if enough restrictions are present. This will be discussed elsewhere. Furthermore, panel models with correlated panel units (e.g. including random time effects  $\tau_t$ ) can be treated by stacking the data in one observation vector (Singer; 2008).

The likelihood of the SEM was transformed explicitly to the prediction error decomposition of Kalman filtering. Both approaches lead to theoretically identical results, but numerical problems occur in the SEM for long time series.

In a second part of the paper (Singer; 2009), the representation of sampled continuous time stochastic processes in terms of the exact discrete model and its representation as SEM is treated.

## Appendix: Numerical considerations

All computations were done using Mathematica 7, which is an interpreter language. The Kalman filter approach is implemented in the LSDE and SDE packages, whereas the SEM computations are obtained with the equations of section 2.<sup>5</sup>

Both the SEM and the SDE approach permit arbitrary nonlinear matrix restrictions, since all system matrices are functions of a parameter vector  $\psi$  (e.g.  $\Sigma_\zeta(\psi)$ ). Using a product of lower triangular matrices  $G(\psi)G'(\psi)$ , a positive semidefinite parametrization is obtained. Likewise, the function  $\frac{1}{2}[c_1 + c_2 + (c_1 - c_2)\tanh(\psi)]$  is in the interval  $(c_1, c_2)$  etc.

In the SEM approach, the structural matrices (of order  $(T + 1)p \times (T + 1)p$ ) are computed automatically by block matrix operations, which may be somewhat tedious in other systems.

The ML estimator was obtained by using a quasi Newton algorithm with BFGS secant updates (Dennis Jr. and Schnabel; 1983) and numerical scores. At the end of the iteration the asymptotic standard errors were computed from the observed Fisher information  $J = -(\partial^2 l / \partial \psi \psi')(\hat{\psi})$ . In the SDE approach, which may be used for time series too, analytical score functions were implemented (Singer; 1990, 1993, 1995).

Generally, in my experience, the SEM approach only works satisfactorily (in terms of numerical stability and speed) if  $(T + 1)p \leq 100$ . The KF approach is only limited by the dimensions  $p$  and  $k$  of the state variables.

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<sup>5</sup>see:

[http://www.fernuni-hagen.de/imperia/md/content/ls\\_statistik/sde.zip](http://www.fernuni-hagen.de/imperia/md/content/ls_statistik/sde.zip),

[http://www.fernuni-hagen.de/imperia/md/content/ls\\_statistik/publikationen/semarchive.exe](http://www.fernuni-hagen.de/imperia/md/content/ls_statistik/publikationen/semarchive.exe)

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